Probability Density Functions of Decaying Passive Scalars in Periodic Domains : An Application of Sinai-Yakhot Theory

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Abstract

Employing the formalism introduced by Sinai and Yakhot [PRL, 63(18), p. 1962, 1989], we study the probability density functions (pdf's) of decaying passive scalars in periodic domains under the influence of smooth large scale velocity fields. The particular regime we focus on is one where the normalized scalar pdf's attain a self-similar profile in finite time, i.e., the so called strange or statistical eigenmode regime. In accordance with the work of Sinai and Yakhot, the central regions of the pdf's are power laws. But the details of the pdf profiles are dependent on the physical parameters in the problem. Interestingly, for small Peclet numbers the pdf's *resemble* stretched or pure exponential functions, whereas in the limit of large Peclet numbers, there emerges a universal Gaussian form for the pdf. Numerical simulations are used to verify these predictions.

1. Introduction

We examine the probability density functions (pdfs) of decaying passive scalars without mean gradients under the action of smooth, incompressible and time aperiodic flows in

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bounded periodic domains. In this situation the evolution of a passive scalar, $\phi(x,y,t)$, is governed by the advection-diffusion (AD) equation.

$$\frac{\partial \phi}{\partial t} + (\vec{u}\cdot\nabla)\phi = \kappa \nabla^2 \phi \tag{1}$$

Here κ represents the molecular diffusivity of the passive scalar and $\vec{u}(x,y,t)$ is the advecting velocity field. The domain (D) under consideration is periodic, specifically we take D to be $[0,2\pi]\times[0,2\pi]$ with opposite sides identified (i.e. a 2-torus).

In this work, we consider time aperiodic velocity fields whose spatial scale of variation is comparable to the scale of the domain. Essentially, the flows are of the type encountered in chaotic advection[1] and the parameters correspond to relatively large Peclet numbers. We focus on the case when the normalized scalar pdf's attain a self-similar profile. This self-similar regime was first described by Pierrehumbert[2],[3] (who named it a strange or statistical eigenmode) and has recently been examined in detail by Fereday and Haynes[4] (hereafter FH) and also by Sukhatme and Pierrehumbert[5] (hereafter SP). The self-similarity of the normalized pdf is indicative of a non-equilibrium steady state. Physically, as was explained in SP and FH, the ingredients in the balance responsible for this state are : (i) a limit on how thin filaments can get (as $\kappa > 0$) and (ii) the "folding and filling" of filaments induced by the finite domain.

To place the things in a proper perspective, we introduce the following scales : L - the scale of the domain, l_v - the scale of variation of the velocity field and $l_s(t)$ - the maximum scale of variation of the scalar field. In terms of these scales the self-similar strange eigenmode is characterized by $l_s(t) \sim l_v \sim$ Ł. Due to this similarity of scales the problem possesses a global nature (see FH and SP). Hence, approximations based on scale separation (such as shifting to a comoving reference frame), which have yielded excellent results in other smooth advection diffusion regimes - sometimes referred to as the Batchelor regime - cannot be fruitfully utilized (see[6],[7] or[8] for a recent review). Also, when $l_s(t) << l_v \sim$ Ł (i.e.,

the Batchelor regime), it has been demonstrated that the pdf's are non-universal, i.e. their shape evolves in time[7]. Obviously, in such a situation there is no limiting scalar pdf and the theory of Sinai and Yakhot[9], which apriori assumes the existence of such a limit, fails.

Indeed, it is the attainment of a self-similar, i.e. limiting, pdf profile in finite time that makes the strange eigenmode regime a suitable candidate for applying the Sinai-Yakhot formalism.

2. The PDF Equation

Consider the dimensionless normalized variable $X = \phi / < \phi^2 >^{1/2}$, by assuming the stationarity in time of $< X^{2n} >$ for all n, Sinai and Yakhot[9] showed,

$$(2n-1) < X^{2n-2} \frac{(\nabla\phi)^2}{Q_1} > = < X^{2n} > \tag{2}$$

where $Q_1 = < (\nabla\phi)^2 >$. Further utilizing Eq. (2), they showed that the pdf of X is given by (denoting the sample space variable by the same symbol),

$$P(X) = \frac{C_1}{g(X)} \exp[-\int_0^X \frac{u}{g(u)} du] \tag{3}$$

where $g(X)$ represents the conditional expectation of the normalized dissipation, i.e $g(X) = < (\nabla\phi)^2 / Q_1 | X >$. As it turns out, later work[10],[11],[12],[13] (see[14] for an overview) clarified that the pdf of any statistically homogenous twice differentiable random field, say $\psi(\vec{x}, t)$, is given by[13],[15],

$$P(\psi, t) = \frac{C_2}{g(\psi, t)/Q_2} \exp[\int_0^\psi \frac{r(u,t)}{g(u,t)} du] \tag{4}$$

$Q_2 = < (\nabla X)^2 >$ and $r(\psi, t) = < (\nabla^2\psi) | \psi >$, $g(\psi, t) = < (\nabla\psi)^2 | \psi >$ represent the conditional diffusion and conditional dissipation respectively. Furthermore, it was shown that if

the moments of $\psi(\vec{x},t)$ are stationary then[15],[16] [1],

$$r(\psi,t) = -\frac{<(\nabla\psi)^2>}{<\psi^2>}\psi \tag{5}$$

Ofcourse, Eq. (5) when substituted in Eq. (4) yields a pdf similar to the Sinai-Yakhot expression, i.e., Eq. (3).

A. Conditional Statistics in the Strange Eigenmode Regime

In the strange eigenmode regime, starting with $l_s(t=0) \sim l_v \sim L$, [2] after a transient period, it is seen that (see SP and FH),

$$<|\phi(x,y,t)|^n> \sim e^{-\alpha_n t} \; ; \; t > T \tag{6}$$

where T represents the duration of the transient period. More importantly, $\alpha_n = n\alpha_1$, this linearity implies the stationarity of the moments of the normalized scalar field [3]. Ofcourse, given the stationarity, we are justified in using Eq. (5), with X replacing ψ. Substituting in Eq. (5) from Eq. (6) we get,

$$r(X,t) = r(X) = -\frac{<(\nabla X)^2>}{<X^2>}X = -\frac{\alpha_2}{2\kappa}X \tag{7}$$

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[1]Ching and Kraichnan[15] hint at the possibility of attaining stationary normalized momemts by utilizing a cyclic domain, the self-similar strange eigenmode appears to be precisely this case.

[2]Other initial conditions, especially $l_s(t=0) << l_v \sim L$ entail an evolution of the scalar field through distinct regimes (see SP and FH for details).

[3]The exponential decay of moments is also valid when $l_s(t) << l_v$, but in this case α_n is a nonlinear function of the moment order n, i.e. the moments are not stationary[7].

Regarding the conditional dissipation, if X and ∇X are independent, then $g(X,t) =< (\nabla X)^2 >$. This coupled with the fact that $g(X,t)$ is even led Sinai and Yakhot to propose the expansion (in the vicinity of $X = 0$)[9],

$$g(X,t) = g(X) =< (\nabla X)^2 > +\beta X^2 + ... \; ; \; \beta = \frac{1}{2}\frac{\partial^2 g}{\partial X^2}|_{X=0} \tag{8}$$

Substituting from Eq. (6), we have (to order X^2),

$$g(X) = \frac{\alpha_2}{2\kappa}(1 + \frac{2\kappa\beta}{\alpha_2}X^2) \tag{9}$$

Furthermore, the normalized conditional diffusion and dissipation are, $R(X) = r(X)/ < (\nabla X)^2 >$ and $G(X) = g(X)/ < (\nabla X)^2 >$ respectively. Using Eq. (7) and Eq. (9),

$$R(X) = -X \quad ; \quad G(X) = 1 + \frac{2\kappa\beta}{\alpha_2}X^2 \tag{10}$$

Recent numerical work (see FH) suggests that, α_2 tends to a non-zero limit as $\kappa \to 0$, hence Eq. (10) gives $G(X) \to 1$ assuming that β does not overwhelm the limit. In other words, keeping the assumption regarding β in mind, X and ∇X tend to become independent as $\kappa \to 0$ and we expect the core of the pdf to tend to a universal Gaussian profile.

Further substituting Eq. (7) and Eq. (9) in Eq. (4) yields (the central part of) the pdf of X to be,

$$P(X) = C_2 \; [1 + \frac{2\kappa\beta}{\alpha_2}X^2]^{-\gamma} \; ; \; \gamma = 1 + \frac{\alpha_2}{4\kappa\beta} \tag{11}$$

Note that, even though the power-law is in agreement with the work of FH, their arguments apply to the tail of the pdf whereas the above expression is valid in the vicinity of $X = 0$. For further elucidation, defining $\delta = 2\kappa\beta/\alpha_2$, let us examine how the shape of $P(X)$ behaves with δ. In terms of δ,

$$P(X) = C_2 \; [1 + \delta X^2]^{-\gamma} \; ; \; \gamma = 1 + \frac{1}{2\delta} \tag{12}$$

For large δ we have $\gamma \to 1$, $\ln(P(X)) \to -\ln(1+\delta X^2)$. As both δ and X are $O(1)$ quantities, all powers of X contribute to $\ln(P(X))$. On the other hand, for small δ we have $\gamma \to 1/2\delta$

and $\ln(P(X)) \sim -X^2/2$, which is the expected outcome from the earlier discussion. Profiles for $\delta = 10, 0.7, 0.001$ are shown in Fig. 1. Note that, as δ decreases $P(X)$ goes from *resembling* a stretched exponential $\rightarrow$ pure exponential $\rightarrow$ (expected) Gaussian function.

3. Numerical Investigation

The AD equation was approximated by a lattice map[3] followed by diffusion in Fourier space. The velocity field is of a single large scale, specifically, we employ the sine flow[17,18],

$$
\begin{aligned}
u(x,y,t) &= f(t)\ A_1\ \sin(y+p_n) \\
v(x,y,t) &= (1-f(t))\ A_2\ \sin(x+q_n)
\end{aligned}
\tag{13}
$$

where $f(t)$ is 1 for $nT \le t < (n+1)T/2$ and 0 for $(n+1)T/2 \le t < (n+1)T$. p_n, q_n ($\in [0, 2\pi]$) are random numbers selected at the beginning of each iteration, i.e., for each period T. A_1, A_2 control the strength of the flow. The flow is implemented as a 2D lattice map $(x_n, y_n) \rightarrow (x_{n+1}, y_{n+1})$[18,3]. A key feature is that the randomness due to p_n, q_n breaks any barriers which may, and generically do, exist in 2D area preserving mappings[19].

A typical example : Starting with a mean zero checkerboard initial condition on a 256×256 grid ($A_1 = A_2 = 2, \kappa = 9.33 \times 10^{-4}$), a typical evolution scenario is shown in Fig. 2. As is seen, the normalized moments attain constant values after a transient period of about 70 iterations [4]. During this transient period $P(X)$ evolves (a remnant of the initial double delta pdf can be seen at iteration 10). Finally, after the moments become

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[4]The transient period may appear large, but it is important to note that the strange eigenmode appears only after the scalar field has folded and filled the domain (see SP and FH for details). Whereas, significant decay of the variance starts much before this time, specifically when the

stationary, $P(X)$ attains a self-similar profile as is seen in lowermost panel of Fig. 2. [5]

Peclet number dependence : To investigate the effect of changing the Peclet number, we run a set of simulations with : (a) fixed flow strength and varying diffusivity and (b) fixed diffusivity and varying flow strengths.

- Varying the diffusivity : Keeping A_1, A_2 fixed and utilizing the same checkerboard initial condition, we vary κ. In each case the evolution of the pdf is similar to that shown in Fig. 2. The pdfs for $\kappa = 2 \times 10^{-3}$ and $\kappa = 5.78 \times 10^{-4}$ in the self-similar stage are displayed in Fig. 3. With respect to the analytical pdf, i.e. Eq. (11), even though β is an unknown the qualitative similarity between Fig. 3 and Fig. 1 is evident (essentially, the dependence of α_2 on κ is fairly weak, when κ changes by an order of magnitude, as in the above simulation, α_2 changes by a much smaller amount). The corresponding plots of the normalized conditional dissipation are shown in Fig. 4. Note that for small κ, we have $G(X) \sim 1$. Also, from Fig. 4 we see that for small κ the range of X is quite small, hence in this situation the Gaussian form describes a fairly large part of the complete pdf. Next, in Fig. 5 we show the pdf's for a number of small diffusivities. Clearly, the core of $P(X)$ tends to a universal Gaussian form.
- Varying the strength of the flow : Fixing $\kappa = 10^{-3}$ we vary A_1, A_2. The decay of the scalar variance for different flow strengths can be seen in Fig. 6. Evidently, $\alpha_2 \propto$ flow

diffusive scale is reached.

[5]It is important to keep in mind that these results are for large Peclet numbers. In fact, in numerical runs with smaller Peclet numbers, even at large times, $< X^{2n} >$ fluctuates with a fairly large amplitude .

strength, therefore for a fixed κ, $\delta \propto 1/(\text{flow strength})$. The implication being that the core of $P(X)$ should tend to a Gaussian function for stronger flows. Fig. 7 shows the pdf's (in the self-similar stage) for two different flow strengths - note the similarity to Fig. 3. Furthermore, Fig. 8 shows the pdf's for a number of simulations with stronger flows. Once again, the emergence of a universal Gaussian core is evident. Also, note the similarity to Fig. 5.

4. Conclusion and Discussion

By applying the formalism introduced by Sinai and Yakhot[9] to a decaying passive scalar obeying the AD equation in a periodic domain, we obtained an expression for the pdf of the normalized scalar field. Broadly categorized as a power-law, the core of the pdf was shown to be dependent on the physical parameters in the AD problem. Moreover, we saw the emergence of a universal Gaussian core for the pdf in : (a) the limit of small diffusivity for a fixed flow strength and (b) the limit of strong flows for fixed κ. Combining these observations we infer the emergence of a universal Gaussian core in the limit of large Peclet numbers. Note that, the detailed dependence on Peclet number is not straight forward as $P(X)$ is a function of both α_2 and κ (Eq. (11)) - in turn α_2 depends on both on κ and flow strength. Interestingly, for smaller Peclet numbers (i.e. larger δ) the power-law pdf profile resembles a pure or stretched exponential function. We believe that this is the reason for the mis-identification of pdf profiles in earlier work[3] (and also SP).

An intriguing, though poorly understood, feature of the strange eigenmode regime is the actual decay rate of the scalar variance - i.e. α_2. Note that, in contrast to the present statistical or strange eigenmode, when the velocity fields are *time periodic*, and $l_s(t) \sim l_v \sim L$, the scalar field represents a periodic eigenfunction of the AD operator. Hence, the structure as well as decay rate of the scalar field are better understood. Regarding these periodic eigenfunctions, or spatially repeating patterns, see[20] for experimental results, SP for a physical

interpretation,[21] for more recent work,[22] for a mathematically rigorous presentation and[23] for an interpretation in terms of the Perron-Frobenius operator induced by the underlying trajectory problem. Also, see[24],[25] for similar ideas in the case of *steady* 3D and 2D flows respectively.

Before concluding we would like to put forth a plausible connection between the eigenmode regime and homogenization theory, with the hope of shedding some light on α_2. Broadly, in the realm of homogenization theory it has been possible to show the convergence, in a coarse grained sense, of the AD equation to a pure diffusion equation for a variety of advecting velocity fields (see Section 2 of[26] or[27] for recent reviews). The most common situation is when $l_v << l_s(t)$, i.e. velocity fields changing rapidly in space but combined with either steadiness or periodicity in time[28],[26]. The opposite limit, along the lines of the work by Kubo[29], is where the velocity fields have longe range spatial correlations but change rapidly in time (see section 2.4.1 of[26] or[27]).

Indeed, it is this second limit where the effective diffusivity of the scalar field is given by the Taylor-Kubo formula[27]. Recent work has shown that such a diffusive limit exists for a broader class of velocity fields, though the formula for the effective diffusivity may not be analytically tractable[30],[31]. Noting the long range spatial ($l_v \sim L$) and short time (randomness at each iteration) correlations of the velocity field required for the emergence of the self-similar eigenmode, we conjecture that the strange eigenmode may be understood as a homogenization phenomenon. Hence, averages such as $< \phi^n >$ obey the diffusion equation, in particular α_2 can be interpreted as an effective diffusivity akin to the Taylor-Kubo formula. Not only does this interpretation lend qualitative support to the observed dependence of α_2 on κ as well as the velocity field, it also implies the linearity of α_n with n.

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FIGURES

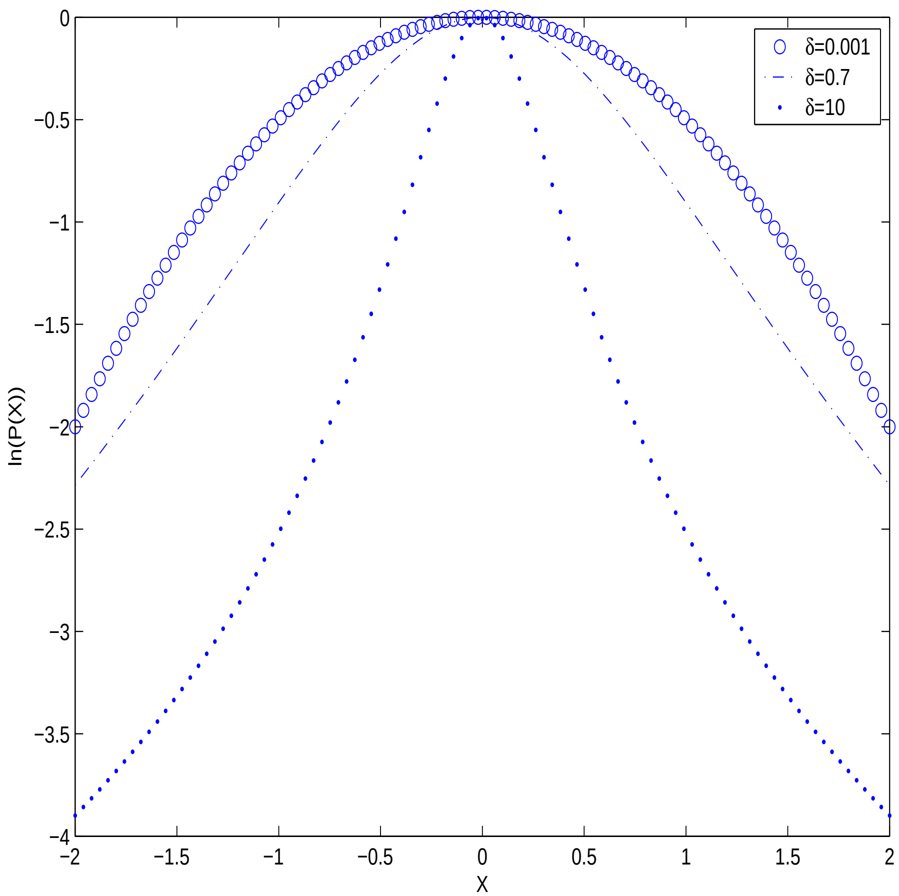

Fig. 1. $\ln(P(X))$ Vs. X from Eq. (11) for differing δ.

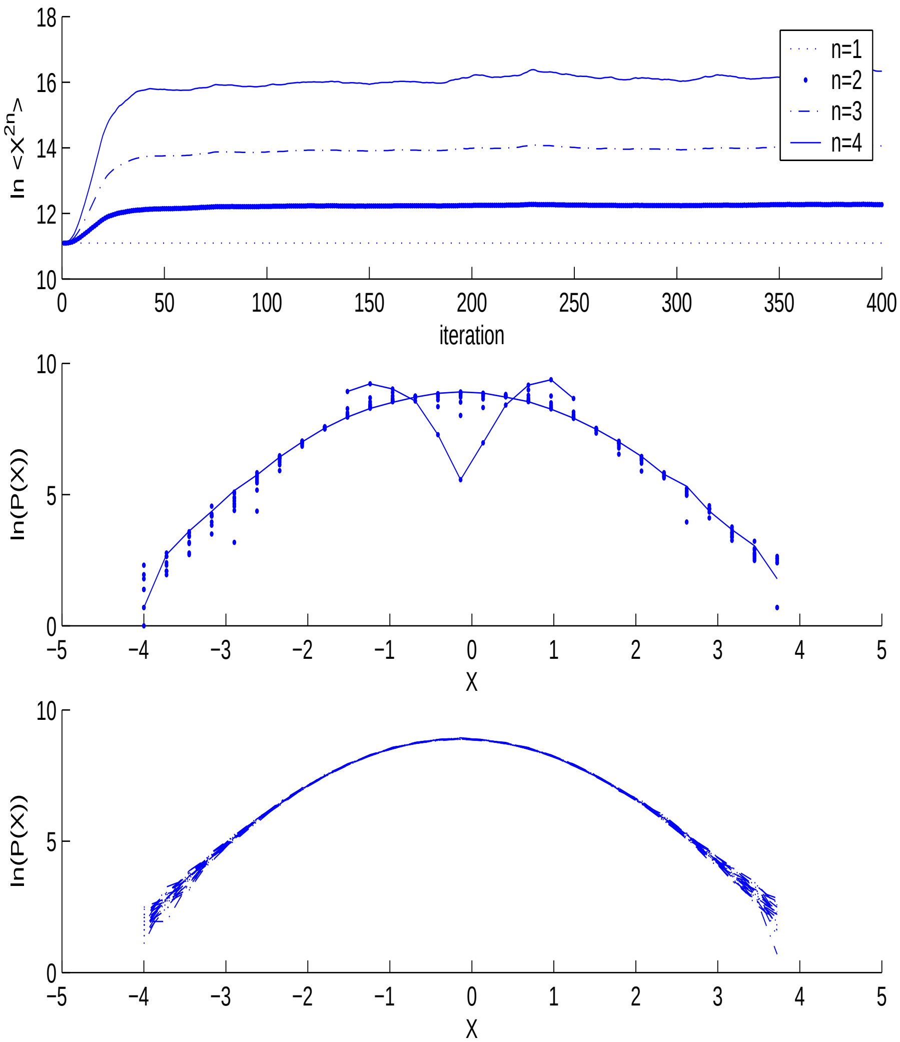

Fig. 2. Typical evolution scenario with $\kappa = 9.33 \times 10^{-4}$. Upper panel shows $\ln(< X^{2n} >)$ Vs. iteration for n=1,2,3 and 4. The middle panel shows the pdf's from iteration 10 to 110 (solid lines at iteration 10 and 110) The lowermost panel shows the pdf's from iteration 150 to 350, i.e. when the normalized moments have become stationary.

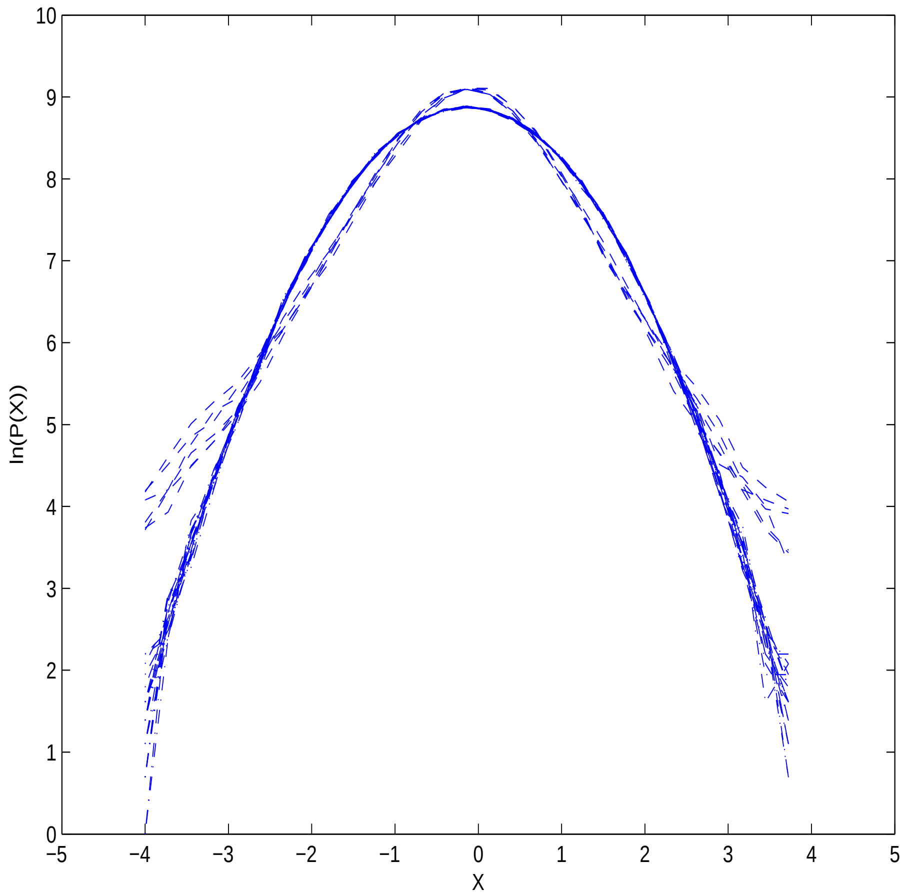

Fig. 3. Self-similar pdf's for $\kappa = 2 \times 10^{-3}$ (dashed), $\kappa = 5.78 \times 10^{-4}$ (solid)

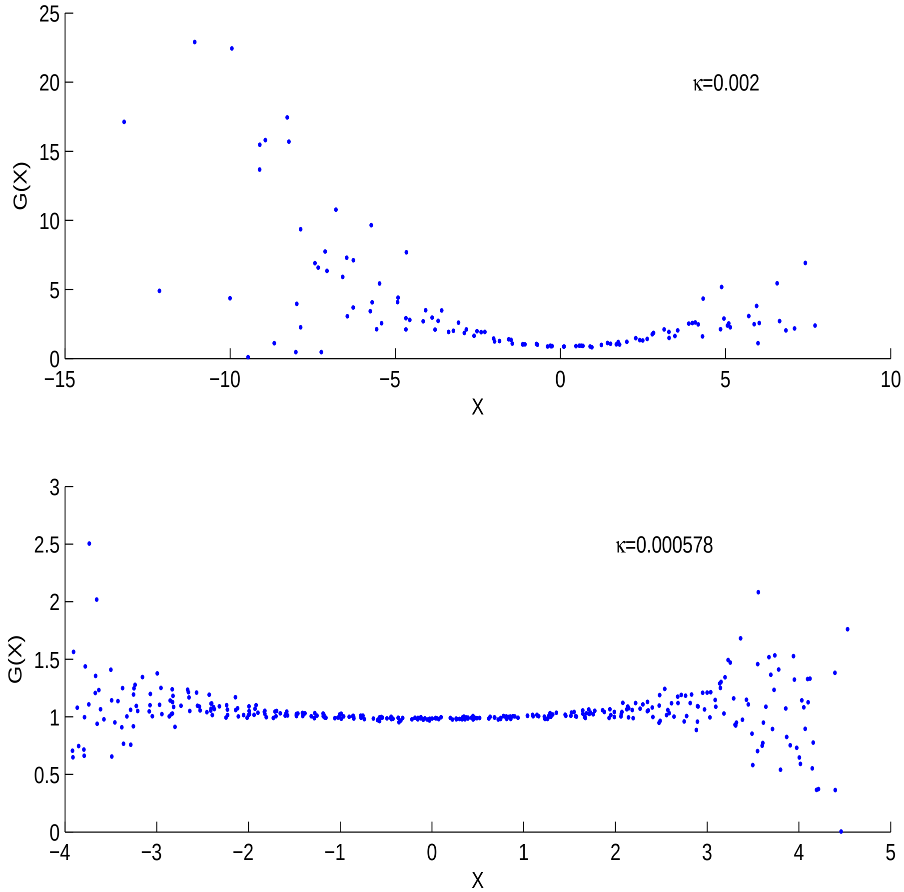

Fig. 4. The normalized conditional dissipation ($G(X)$) Vs. X for the same set of diffusivities as in Fig. 3. Note the range of the axes in the two subplots.

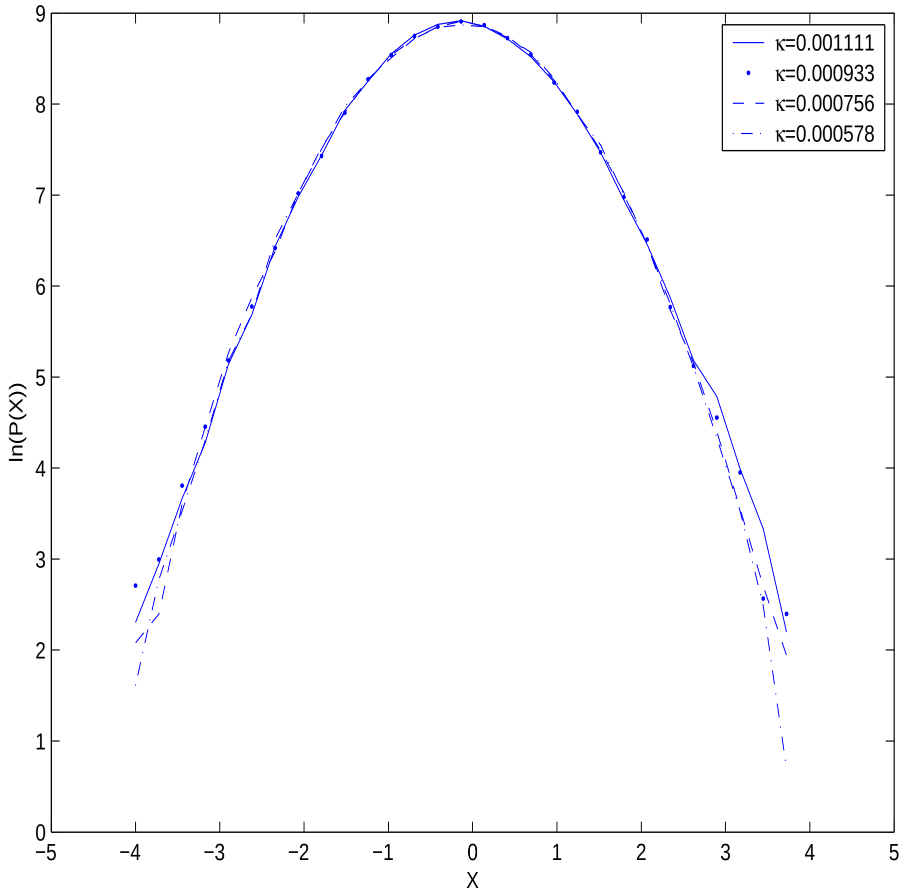

Fig. 5. pdfs for $\kappa = 1.11 \times 10^{-3}, 9.33 \times 10^{-4}, 7.56 \times 10^{-4}, 5.78 \times 10^{-4}$: The emergence of a universal Gaussian core.

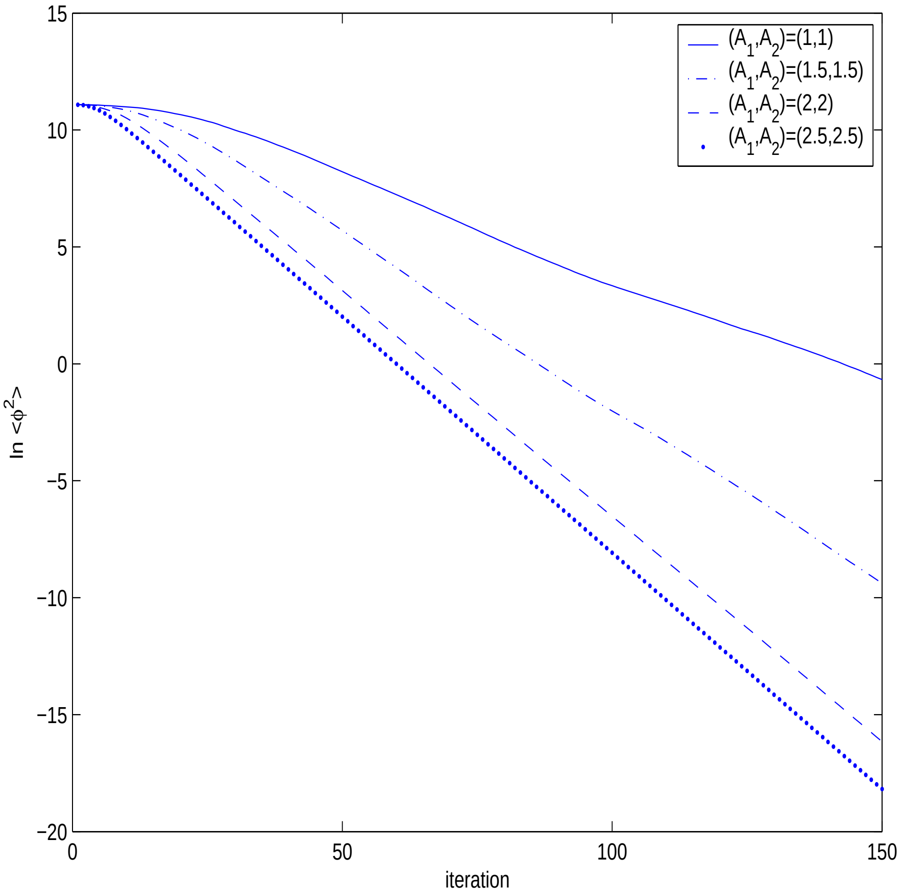

Fig. 6. Decay of the variance with fixed κ and varying flow strengths. Clearly, $\alpha_2 \propto$ (flow strength).

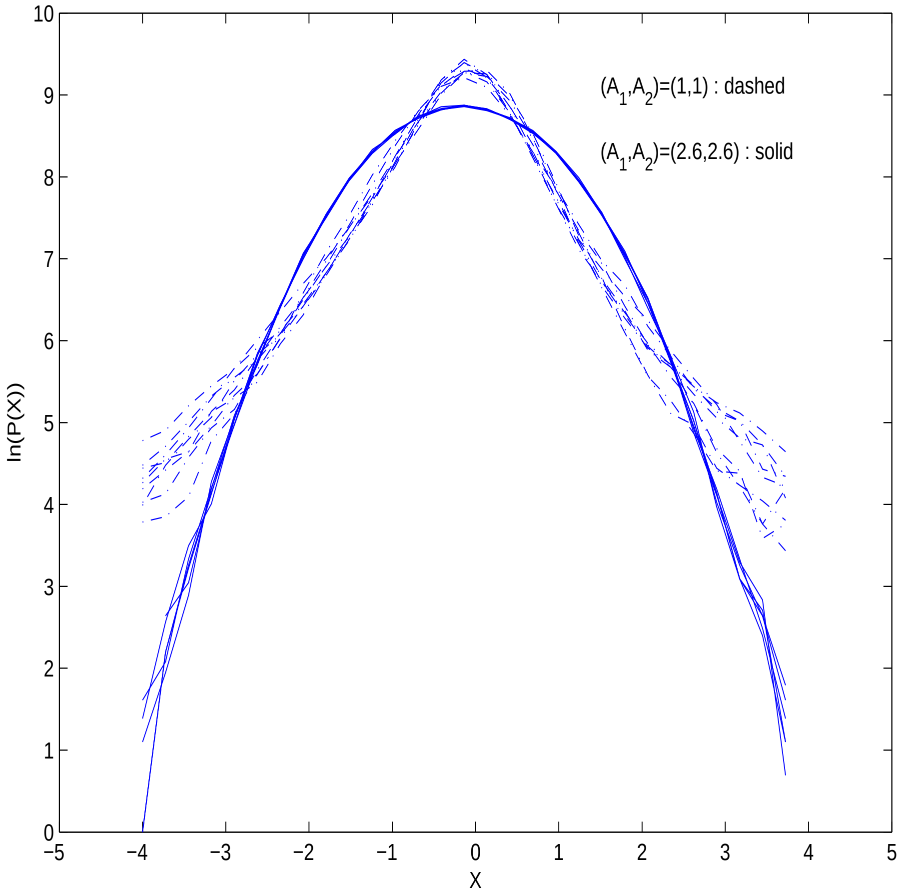

Fig. 7. $\ln(P(X))$ Vs. X in the self-similar stage for $(A_1, A_2) = (1, 1)$ (dashed curves) and $(A_1, A_2) = (2.6, 2.6)$.

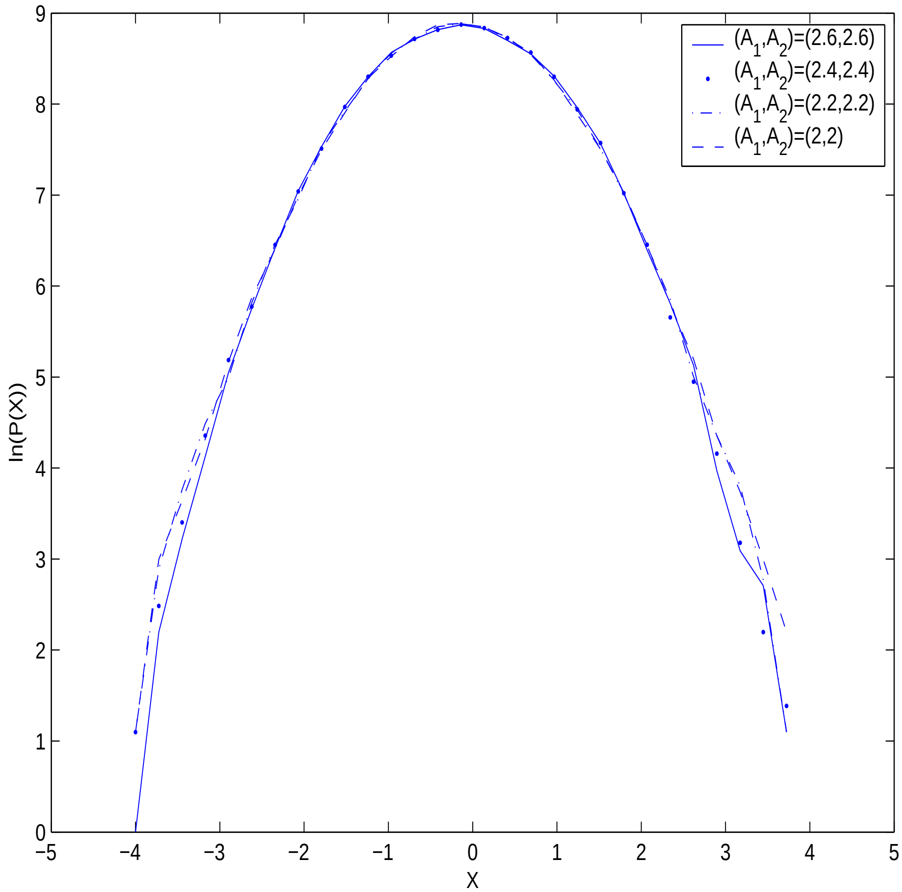

Fig. 8. pdfs for $(A_1, A_2) = (2, 2)$, $(A_1, A_2) = (2.2, 2.2)$, $(A_1, A_2) = (2.4, 2.4)$ and $(A_1, A_2) = (2.6, 2.6)$. Once again, note the emergence of a universal Gaussian core.